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Industrial polymers classification using laser-induced breakdown spectroscopy combined with self-organizing maps and K-means algorithm

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ABSTRACT

To extend the industrial polymer species classification and improve its efficiency. Laser-induced breakdown spectroscopy (LIBS) combined with unsupervised learning algorithms of self-organizing maps (SOM) and K-means was employed to differentiate industrial polymers in the open air. Only the intensities of non-metallic lines, including two molecular band lines (C-N(0,0) 388.3 nm and C_2(0,0) 516.5 nm) and four atomic emission lines (C I 247.9 nm, H I 656.3 nm, N I 746.9 nm and O I 777.3 nm) were used. Firstly, the SOM neural network with adjusting spectral weightings (ASW) was applied to separate 20 kinds of polymers preliminarily. The results were obtained in the output space which indicated that 18 kinds of polymers have been separated except for polycarbonate (PC) and polystyrene (PS). Afterwards, the K-means clustering algorithm was utilized to separate PC and PS. The accuracy of the industrial polymers classification for 20 kinds of polymers was 99.2%. It demonstrated that the feasibility of clustering of industrial polymers using LIBS.

1. Introduction

The recycling of waste industrial polymers is an increasingly important issue to solve the ecological environment pollution and save precious resources, such as air, soil, and water [1,2]. Identification and classification are crucial stages in the recycling of the waste polymers. The manual sorting methods based on labels are costly and still cannot ensure high accuracy. Several technologies have been proposed for the fast identification of plastic wastes. Raman spectroscopy, near-infrared spectroscopy (NIR) and x-ray fluorescence (XRF) spectroscopy have been used. Raman spectroscopy distinguishes plastic types on the basis of molecular structure detected by the scattered light of sample surface, while the technology has a deficiency in detective sensitivity [3]. NIR determines the structure of targets by detecting near-infrared region (from 780 nm to 2526 nm) of the absorption spectrum [4]. Nonetheless, it is arduous for this technology to identify black polymers or polymers with the dusty surface. And the signal is dependent on pollution of the sample surface [5]. XRF is applied to recognize polyvinyl chloride

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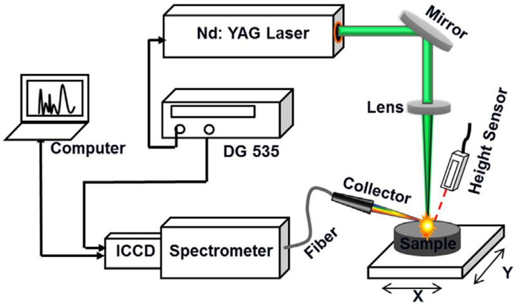

Fig. 1. Schematic diagram of the experimental setup.

(PVC) via detecting chlorine atoms, as it is not sensitive to light elements [6]. Accordingly, an efficient online technology for plastic classification is urgently needed to make up for the deficiencies of these technologies above.

Laser-induced breakdown spectroscopy (LIBS) [7–10], with its attractive advantages of no or simple sample preparation, remote and *in-situ* measurement capability, multi-elemental analysis and nearly non-destruction combined with stoichiometry have been studied by many researchers for polymer classification [11–17]. Boueri et al. [18] have used LIBS with the artificial neural network (ANN), to identify eight kinds of polymers with 14 spectral lines including metallic elements and non-metallic elements lines. Banaee et al. [12] applied discriminant function analysis (DFA) with 10 spectral lines to identify and classify 6 groups of the most used polymers materials. Grégoire et al. [19] used C_2 signal to differentiate aliphatic and aromatic polymers and adopted line ratios, principal component analysis (PCA) and partial least squares regression (PLSR) to classify other polymers. Yu et al. [20] identified 11 kinds of polymers using support vector machine (SVM) with 16 spectral lines under argon background. Costa et al. [21] adopted k-nearest neighbors (KNN) and soft independent modeling of class analogy (SIMCA) to classify 6 kinds of polymer e-waste, and the average accuracies were 98% and 92%, respectively. Studies mentioned above had obtained good results on the classification of polymers using LIBS with various of stoichiometry methods. However, most of these previous researchers always adopted metallic and non-metallic lines simultaneous, as is well known, metallic elements are from the additives in polymers, which usually varied in species and contents, even some polymers without additives. Therefore, the industrial polymer species classification will be limited if the characteristic spectral lines of additives were used. In addition, most of these works used supervised learning algorithms, such as ANN, DFA, and SVM, which need prior knowledge of the dataset and the number of plastics types, in general, must be specified in advance.

To extend the industrial polymer species classification and improve its efficiency, LIBS combined with unsupervised learning algorithms of SOM and K-means was employed to differentiate industrial polymers in the open air. Only 6 non-metallic spectral lines were chosen for distinguishing 20 industrial polymers. In this work, the SOM neural network with adjusting spectral weightings (ASW) was applied to separate 20 kinds of polymers preliminarily; then the cluster analysis was achieved by an iterative process, where the mean error of clustering was used as the criterion. Afterwards, the K-means clustering algorithm was utilized to separate remaining unseparated polymers.

2. Experiments and methods

2.1. Experimental setup and samples

Fig. 1 shows the schematic representation of the experimental setup. A second harmonic Q-Switched Nd:YAG pulsed laser operating at 532 nm (pulse duration 6 ns, repetition rate 10 Hz, pulse energy 40 mJ) was used in open air. The laser beam was reflected by a dichroic mirror and focused onto the surface of polymer samples perpendicularly by a lens with a focal length of 150 mm. The plasma emission was collected by a light collector and then was coupled into an echelle spectrometer (Andor Tech., Mechelle 5000, spectral range from 230 nm to 850 nm, resolution $\lambda/\Delta\lambda = 5000$) by a fiber. The spectrometer was equipped with an ICCD (Andor Tech., iStar DH-334T). A digital delay generator (DG535) synchronously controlled the ICCD operated in the gated mode and the laser output. The sample was placed on a platform and controlled by a computer. A height sensor was used to monitor the sample height. The samples used in this work contain 20 industrial polymers and their physical property is presented in Table 1.

2.2. Experimental method and selection of characteristic spectral lines

The atomic spectral lines of carbon (C), hydrogen (H), oxygen (O), and nitrogen (N) were selected as analytical lines to optimize experimental parameters. To obtain high spectral intensity and the signal-to-background ratio (SBR), the gate delay time and width were optimized firstly. The best gate delay time and width of the ICCD were 2.5 and 2 μs, respectively. To prevent air breakdown occurring, the focal point was under the target surface at a depth of 1.5 mm. In the experiment, to reduce the influence of the laser energy fluctuation on the spectral intensity, an integration time was set to 3 s per spectrum,